The E3SM Nonhydrostatic Dynamical Core

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PDEs on the sphere, Montreal, 2019
E3SM: Energy Exascale Earth System Model

- 8 DOE labs + universities. Total ~50 FTEs spread over 80 staff
- Atmosphere, Land, Ocean and Ice component models
- Development driven by DOE-SC mission interests: Energy/water issues looking out 40 years
- **Key computational goal:** Ensure E3SM will run well on upcoming DOE pre-exascale and exascale computers
- [https://github.com/E3SM-Project/E3SM](https://github.com/E3SM-Project/E3SM)
- [http://e3sm.org](http://e3sm.org)
E3SM Component Models

- **Atmosphere:** EAM
  - Branched from CESM’s CAM5
  - HOMME dycore
- **Land:** ELM
  - Branched from CESM’s CLM4.5
- **Ocean:** MPAS-O
- **Sea Ice:** MPAS-SI
- **Land Ice:** MPAS-LI
HOMME-NH New features / highlights

- **HEVI-IMEX. (A. Steyer’s talk)**
  - New high stage IMEX methods optimized for CFL
  - Laprise formulation + static condensation: single implicit equation for geopotential height

- **Interpolatory SL Transport + property preservation (O. Guba’s poster)**
  - Very efficient scheme, with conservation, monotonicity and consistency imposed with single all-reduce style tree-code.

- **HOMMEXX**
  - Rewrite in C++/kokkos, for GPU performance
  - Bertagna et al., GMD 2019

- **Energy Conservation**
  - Lorenz staggering, Mimetic SE (horizontal) + SB81 (vertical)
  - Discrete produce rule in the vertical – allows for more flexibility for energy conserving formulations

- **Pressure Gradient Errors**
  - Large improvements over original HOMME hydrostatic implementation
HOMME-NH

- Laprise mass coordinate formulation
- Shallow atmosphere
- Lorenz staggering in the vertical
- Mimetic vertical differencing (Simmons & Burridge MWR 1981)
- SE mimetic horizontal differencing (Taylor & Fournier, JCP, 2010)
- Vertically Lagrangian (SJ Lin, MWR 2004)
- Diagnostic equations (quadrature rules from CCM3 tech. report, 1996)
Energy Conservation 1

• Use Hamiltonian form of the equations and mimetic methods to ensure term-by-term balance in energy budget
  – No spurious sources of energy from discretization error
  – Found to be more stable and robust in hydrostatic HOMME. (Taylor & Fournier JCP 2010)
  – E.g.: HOMME, TRSK, Gungho FE, DYNAMICO, etc…
  – Used as guiding principal in development of HOMME-NH
In the shallow water equations, energy conservation via mimetic methods is equivalent to *entropy stabilization*:

- Shown to stabilize high order methods for a wide variety of applications:
  - Winters et al., JCP 2018, Fisher & Carpenter JCP 2013
  - Especially important for high order methods which are prone to being nonlinearly unstable due to aliasing errors
  - Strong connection between aliasing errors and discrete product and chain rules (Gassner, ICOSAHOM 2018)
Energy Conservation 3

• Salmon, J. Atmos. Sci. 2006:
  ― “From the standpoint of differential equations, conservation laws arise from manipulations that typically include the product rule for derivatives. Unfortunately, the product rule does not generally carry over to discrete systems; try as we might, we will never get digital computers to respect it.”
  ― Product rule: \( d(ab)/dx = b \, da/dx + a \, db/dx \)
  ― Mimetic methods: discrete integration by parts makes up for the lack of a discrete product rule.
SB81 product rule

Average interfaces to midpoints:
\[ \bar{\phi}_i = \frac{1}{2} \left( \phi_{i+1/2} + \phi_{i-1/2} \right) \]

Average midpoints to interfaces (and extrapolate to the boundaries)
\[ \bar{p}_{i+1/2} = \frac{(p\Delta \eta)_{i+1} + (p\Delta \eta)_i}{2\Delta \eta_{i+1/2}} \quad \bar{p}_{1/2} = p_1 \quad \bar{p}_{n+1/2} = p_n \]

Derivative of midpoint quantity at interfaces:
\[ \left( \frac{\partial p}{\partial \eta} \right)_{i+1/2} = \frac{p_{i+1} - p_i}{\Delta \eta_{i+1/2}} \]

Derivative of interface quantity (one sided at boundaries)
\[ \left( \frac{\partial \phi}{\partial \eta} \right)_i = \frac{\phi_{i+1/2} - \phi_{i-1/2}}{\Delta \eta_i} \]
SB81 Discrete Product Rule

Product rule for interface quantities -> midpoints

\[
\left( \frac{\partial}{\partial \eta} (ab) \right)_i = \bar{b} \left( \frac{\partial a}{\partial \eta} \right) + \bar{a} \left( \frac{\partial b}{\partial \eta} \right)
\]

Product rule for midpoint quantities -> interfaces

\[
\left( \frac{\partial}{\partial \eta} (cd) \right)_{i+1/2} = \left( \frac{d}{\Delta \eta_i} \right) \Delta \eta_{i+1/2} \left( \frac{\partial c}{\partial \eta} \right) + \left( \frac{c}{\Delta \eta_i} \right) \Delta \eta_{i+1/2} \left( \frac{\partial d}{\partial \eta} \right)
\]

- Considered impossible to unstructured grids in two or more dimensions.
- Gives us more flexibility when formulating the equations for energy conservation.
NH Equations – Laprise Formulation

\[
\frac{\partial \mathbf{u}}{\partial t} + (\nabla_\eta \times \mathbf{u} + 2\mathbf{\Omega}) \times \mathbf{u} - w \nabla_\eta w + \frac{1}{2} \nabla_\eta K + \dot{\eta} \frac{\partial \mathbf{u}}{\partial \eta} + c_p \theta_v \nabla_\eta \Pi + \frac{\partial p}{\partial \pi} \nabla_\eta \phi = 0
\]

\[
\frac{\partial w}{\partial t} + \mathbf{u} \cdot \nabla_\eta w + \dot{\eta} \frac{\partial w}{\partial \eta} + g - g \frac{\partial p}{\partial \pi} = 0
\]

\[
\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla_\eta \phi + \dot{\eta} \frac{\partial \phi}{\partial \eta} - gw = 0
\]

\[
\frac{\partial}{\partial t} (\Theta + \nabla_\eta \cdot (\Theta \mathbf{u})) + \frac{\partial}{\partial \eta} (\Theta \dot{\eta}) = 0
\]

\[
\frac{\partial}{\partial t} \left( \frac{\partial \pi}{\partial \eta} \right) + \nabla_\eta \cdot \left( \frac{\partial \pi}{\partial \eta} \mathbf{u} \right) + \frac{\partial}{\partial \eta} \left( \frac{\partial \pi}{\partial \eta} \dot{\eta} \right) = 0
\]

\[
\Theta = \frac{\partial \pi}{\partial \eta} \theta_v \\
\text{EOS: } \frac{\partial \phi}{\partial \eta} = -R\Theta \frac{\Pi}{p}
\]
Energy Conservation: Validation

- DCMIP2012 test 4: Jablonowski & Williamson baroclinic instability running on a small (x1000) planet
- Run to day 30, then restart with viscosity turned off and look at energy budget as function of timestep
- Total Energy Conservation: converges O($dt^3$) to machine precision
- Only dissipation should be from time discretization error: measured KE, IE, and PE dissipation rates should converge to zero as O($dt$)
Pressure Gradient Treatment
DCMIP 2012 Test 2.0

• Atmosphere at rest, non-rotating planet, Schar-like circular mountain (Schar et al., MWR 2002)
• Switching to Exner based pressure gradient and prognostic potential temperature reduces dispersion errors (Thuburn, QJRMS, 2006; Toy & Randall, JCP 2007)
• HOMME-NH Results for different energy conserving pairs:
  – (prognostic variable, pressure gradient form)
  – Pairs are chosen so that the transfer of KE->IE from the pressure gradient will exactly cancel the transfer of IE->KE from the thermodynamic equation when using a mimetic discretization
DCMIP 2012 Test 2-0: Shar mountain on the sphere

\[ T, \quad (1/\rho) \nabla p \]

\[ \rho \theta, \quad c_p \theta \nabla \Pi \]

\[ \theta, \quad c_p (\nabla (\theta \Pi) - \Pi \nabla \theta) \]

Entropy: \[ \eta, \quad c_p (\nabla (\theta \Pi) - \Pi \theta \nabla \eta) \]
Held-Suarez Test Case + Topography

- Run for 1600d, average over last 1000d
- 1° horizontal resolution (ne=30), 26 levels
- Modifications:
  - Use realistic topography
  - For NH model, apply velocity drag term to all three velocity components

\[
\frac{\partial v}{\partial t} = -k_v(\sigma)v
\]
\[
\frac{\partial T}{\partial t} = -k_T(\phi, \sigma)[T - T_{eq}(\phi, \sigma)]
\]

\[
T_{eq} = \max \left[ 200K, \left[ 315K - (\Delta T)_y \sin^2 \phi - (\Delta \theta)_z \log \left( \frac{p}{p_0} \right) \cos^2 \phi \right] \left( \frac{p}{p_0} \right)^\kappa \right]
\]

\[
k_T = k_a + (k_s - k_a) \max \left( 0, \frac{\sigma - \sigma_b}{1 - \sigma_b} \right) \cos^4 \phi
\]

\[
k_v = k_i \max \left( 0, \frac{\sigma - \sigma_b}{1 - \sigma_b} \right)
\]

- \( \sigma_b = 0.7 \)
- \( k_i = 1 \text{ day}^{-1} \)
- \( k_a = \frac{1}{40} \text{ day}^{-1} \)
- \( k_s = \frac{1}{4} \text{ day}^{-1} \)
- \( (\Delta T)_y = 60K \)
- \( (\Delta \theta)_z = 10K \)

\[
p_0 = 1000 \text{ mb}
\]
\[
\kappa = \frac{R}{c_p} = \frac{2}{7}
\]
\[
c_p = 1004 \text{ J kg}^{-1} \text{ K}^{-1}
\]

\[
\Omega = 7.292 \times 10^{-5} \text{ s}^{-1}
\]
\[
g = 9.8 \text{ m s}^{-2}
\]
\[
a_e = 6.371 \times 10^6 \text{ m}
\]
Climatology w/topography

HOMME

Zonal-mean Temperature degrees kelvin

Zonal-mean Zonal Wind meters/second

Temperature Eddy Variance $K^2$

HOMME-NH (H)

Zonal-mean Temperature degrees kelvin

Zonal-mean Zonal Wind meters/second

Temperature Eddy Variance $K^2$

HOMME-NH

Zonal-mean Temperature degrees kelvin

Zonal-mean Zonal Wind meters/second

Temperature Eddy Variance $K^2$
Divergence – Climatology

HOMME
Climatology 788hPa

HOMME-NH (H)
Climatology 788hPa

HOMME-NH
Climatology 788hPa

Divergence 1/s

-4e-05 -3e-05 -2e-05 -1e-05 0 1e-05 2e-05 3e-05 4e-05

Climatology 788hPa
Summary

• Energy conservation (or entropy stabilization) is a useful guiding principle for choice of discretization and equation formulation, especially for high order methods

• Potential temperature / Exner pressure formulation significantly improves SE response to topography
  – Should allow HOMME-NH to reduce divergence damping, or use rougher topography

500mb specific humidity in the DCMIP 2016 baroclinic instability (Ullrich et al. 2013) test case with Reed & Jablonowski (2012) idealized physics running at 3km horizontal resolution. Used to test parallel scalability and performance of HOMME-NH